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=> fil cap
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FILE LAST UPDATED: 15 Feb 2007  (20070215/ED)

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=> d que l4
L1                STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str
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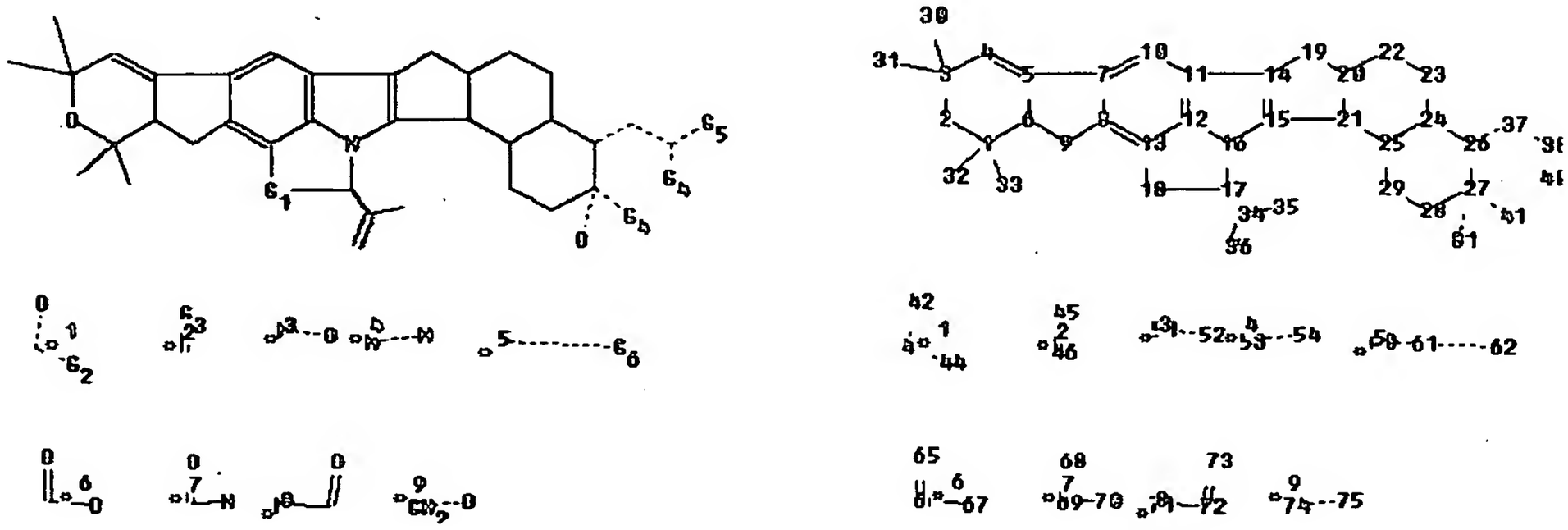

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chain nodes :
30  31  32  33  34  35  36  39  40  41  42  43  44  45  46  51  52  53  54  60  61
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62 65 66 67 68 69 73 74 75 81
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29
ring/chain nodes :
37 38 70 71 72
chain bonds :
1-32 1-33 3-30 3-31 17-34 27-81 34-35 34-36 38-39 42-43 43-44 45-46 51-
52
53-54 60-61 61-62 65-66 66-67 68-69 69-70 72-73 74-75
ring/chain bonds :
26-37 27-41 37-38 38-40 71-72
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 7-10 8-9 8-13 10-11 11-12 11-14
12-13 12-16 13-18 14-15 14-19 15-16 15-21 16-17 17-18 19-20 20-21 20-22
21-25 22-23
23-24 24-25 24-26 25-29 26-27 27-28 28-29
exact/norm bonds :
1-2 1-6 1-32 1-33 2-3 3-4 3-30 3-31 4-5 5-6 5-7 6-9 8-9 11-14 12-16
13-18 14-15 14-19 15-16 15-21 16-17 17-18 17-34 19-20 20-21 20-22 21-25
22-23 23-24
24-25 24-26 25-29 26-27 26-37 27-28 27-41 27-81 28-29 34-35 34-36 37-38
38-39 38-40
42-43 43-44 45-46 51-52 53-54 60-61 61-62 65-66 66-67 68-69 69-70 71-72
72-73 74-75
normalized bonds :
7-8 7-10 8-13 10-11 11-12 12-13

G1:[*1],[*2]

G2:H,Cy,Ak

G3:[*3],[*4]

G4:H,O

G5:CHO,[*5]

G6:CN,[*6],[*7],[*8],[*9]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:CLASS
31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS
43:CLASS 44:CLASS 45:CLASS 46:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS
60:CLASS 61:CLASS
62:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS
72:CLASS 73:CLASS
74:CLASS 75:CLASS 81:CLASS

L3 13 SEA FILE=REGISTRY SSS FUL L1
L4 5 SEA FILE=CAPLUS ABB=ON PLU=ON L3

=> d l4 ibib abs hitstr tot

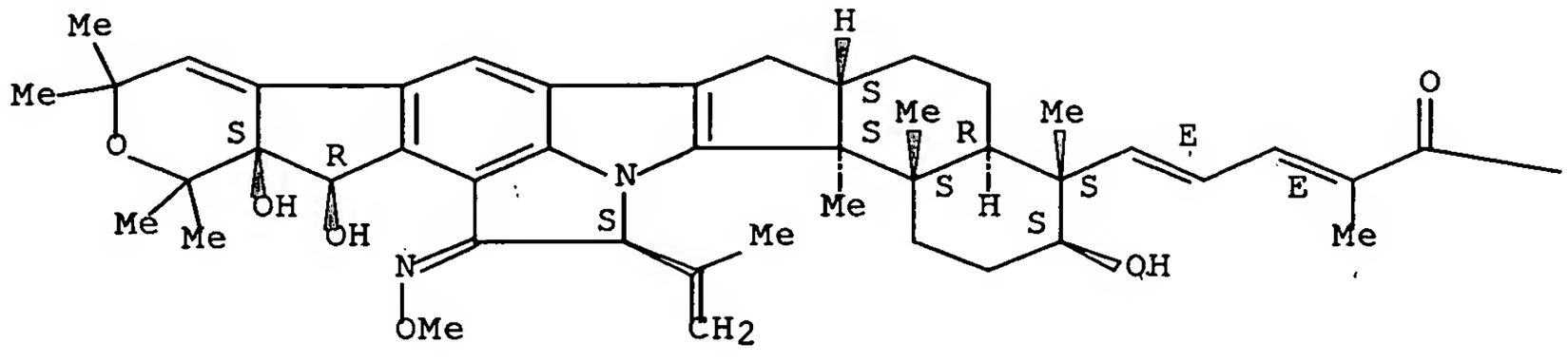
L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:406882 CAPLUS Full-text
DOCUMENT NUMBER: 137:288491
TITLE: Comparison of nodulisporic acid analogs in a Lucilia sericata in vitro assay and a Ctenocephalides felis membrane feeding system
AUTHOR(S): Felcetto, T.; Ondeyka, J.; Colletti, S. L.; Meinke, P. T.; Shoop, W. L.
CORPORATE SOURCE: Merck Research Laboratories, Merck and Co., Inc., Rahway, NJ, 07065, USA
SOURCE: Journal of Parasitology (2002), 88(2), 223-226
CODEN: JOPAA2; ISSN: 0022-3395
PUBLISHER: American Society of Parasitologists
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A medicinal chemical program on the nodulisporic acid chemical class, guided by an artificial membrane flea-feeding assay, has recently identified permissive and nonpermissive regions of the pharmacophore for exploitation against fleas. This pathway was validated when several promising compds. from this program were administered orally to dogs at 15.0 mg/kg and found to have >90% flea activity for 2 wk. To determine if a surrogate insect assay would have provided the same guidance, a nodulisporic acid analog series was examined in both a Lucilia sericata larval assay and an artificial membrane flea-feeding assay using Ctenocephalides felis. Results from both insect assays were concordant in that even subtle chemical modification or substitution to the left-hand side of the nodulisporic acid pharmacophore resulted in substantial loss of insecticidal activity. Both assays were also in general agreement that the only modifications to the pharmacophore that did not result in loss of activity occurred to the C-8 side chain on the right-hand side of the mol. Although there was good agreement between the 2 assays on the general regions of the pharmacophore, there was variance on individual compds. in the mono- and disubstituted amide series from the C-8 side chain. For example, the L. sericata assay showed several analogs from this subclass to possess similar activity to the parent acid, whereas the membrane assay indicated superior activity against fleas relative to the same parent. Consequently, although there was substantial general agreement between the assays, it was concluded that finer optimization of a lead compound should be done against the target parasite, even if it is ex vivo, as early as possible in a medicinal chemical program.

IT ***470460-65-2***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comparison of nodulisporic acid analogs in a Lucilia sericata in vitro assay and a Ctenocephalides felis membrane feeding system)
RN 470460-65-2 CAPLUS
CN 2,4-Pentadienamide, N-(1,1-dimethylethyl)-5-[(3S,4S,4aR,6aS,12aS,13R,15S,16bS,16cS)-2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,12a,13-trihydroxy-14-(methoxyimino)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-, (2E,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.

PAGE 1-A



PAGE 1-B

—NHBu-t

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:719716 CAPLUS Full-text
DOCUMENT NUMBER: 134:67446
TITLE: Chemical modification of nodulisporic acid A: preliminary structure-activity relationships
AUTHOR(S): Meinke, P. T.; Ayer, M. B.; Colletti, S. L.; Li, C.; Lim, J.; Ok, D.; Salva, S.; Schmatz, D. M.; Shih, T. L.; Shoop, W. L.; Warmke, L. M.; Wyvratt, M. J.; Zakson-Aiken, M.; Fisher, M. H.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065-0900, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(20), 2371-2374
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Medicinal chemical efforts were initiated to identify the key constituents of the nodulisporic acid A pharmacophore that are integral to its potent insecticidal activity. New semisynthetic derivs. delineated nodulisporic acid A into 'permissive' and 'nonpermissive' regions and led to the discovery of new nodulisporamides with significantly improved flea efficacy.

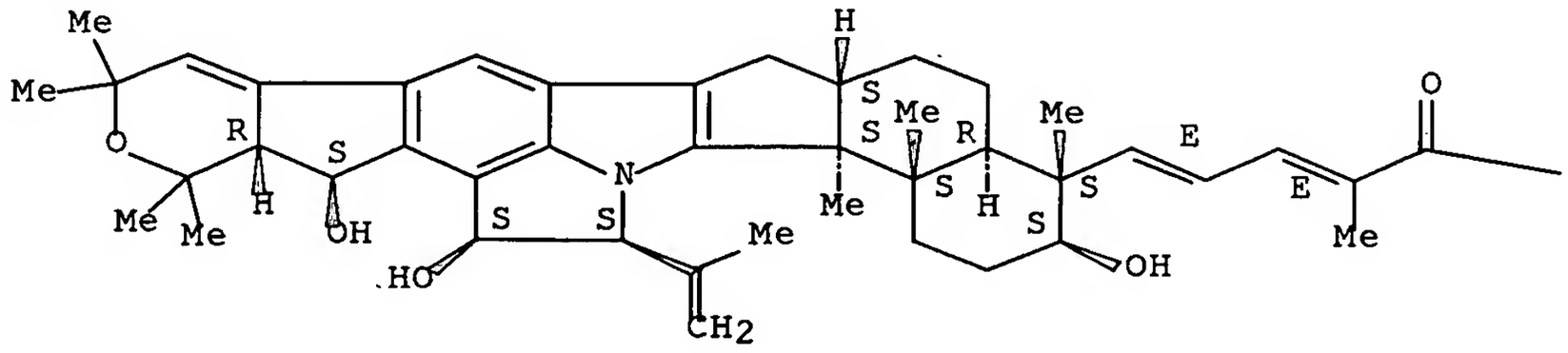
IT ***315716-15-5***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and structure-activity relationship of nodulisporamides as systemic insecticides for flea infestation)

RN 315716-15-5 CAPLUS

CN 2,4-Pentadienamide, 5-[(3S,4S,4aR,6aS,12aR,13S,14S,15S,16bS,16cS)-2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-N,2-dimethyl-, (2E,4E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

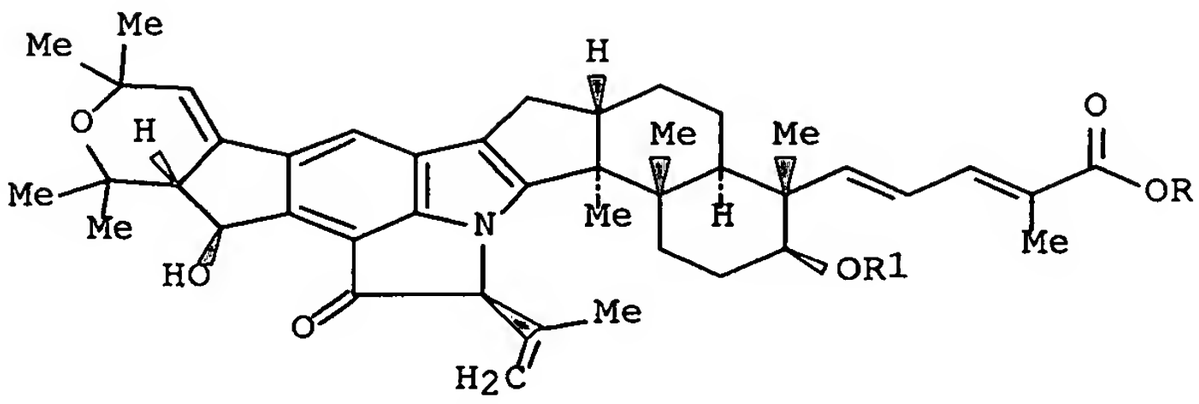


PAGE 1-B

—NHMe

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:606732 CAPLUS Full-text
DOCUMENT NUMBER: 127:275095
TITLE: Nodulisporic Acid A, a Novel and Potent Insecticide from a Nodulisporium Sp. Isolation, Structure Determination, and Chemical Transformations
AUTHOR(S): Ondeyka, John G.; Helms, Gregory L.; Hensens, Otto D.; Goetz, Michael A.; Zink, Deborah L.; Tsipouras, Athanasios; Shoop, Wesley L.; Slayton, Lyndia; Dombrowski, Anne W.; Polishook, Jon D.; Ostlind, Dan A.; Tsou, Nancy N.; Ball, Richard G.; Singh, Sheo B.
CORPORATE SOURCE: Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Journal of the American Chemical Society (1997), 119(38), 8809-8816
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I R=R1=H
II R=Me, R1=H
III R=Me, R1=p-bromobenzoyl

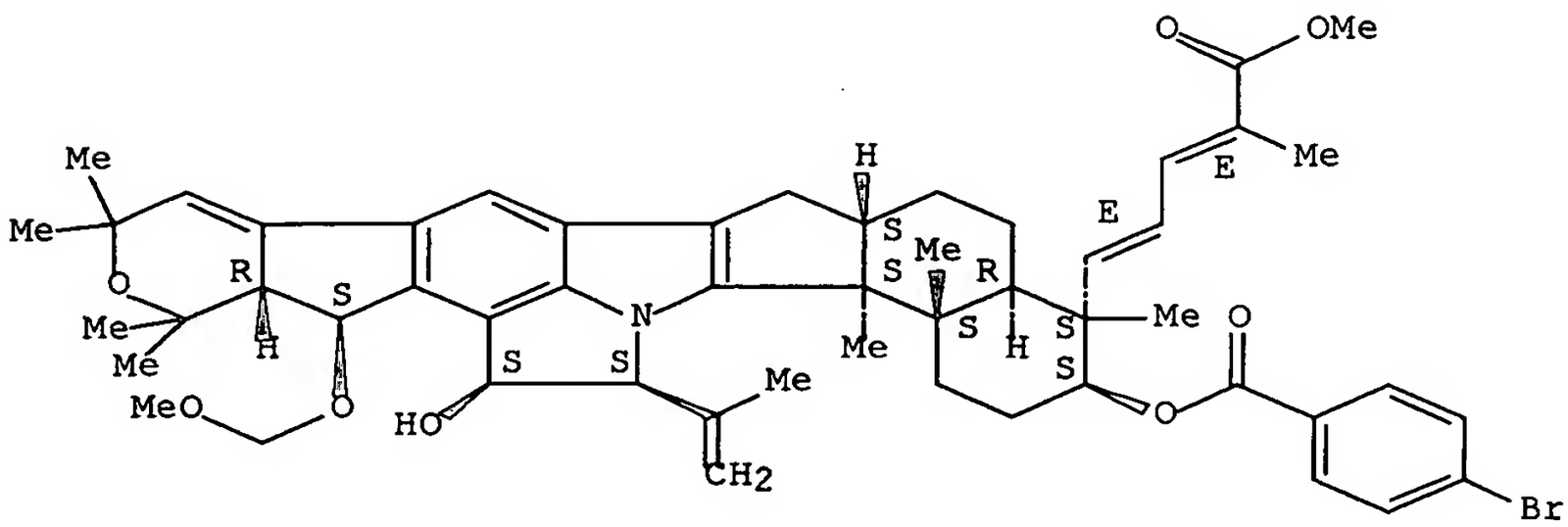
AB The potent insecticidal agent nodulisporic acid A (I), representative of a new class of indole terpenes, was isolated from fermns. of a Nodulisporium sp. Nodulisporic acid A was active against the larvae of the blowfly and mosquito at sub-part-per-million levels. The structure followed mainly from a consideration of spectroscopic evidence, including Dunkel's computerized 2D INADEQUATE anal. The relative stereochem. of the eastern and western hemispheres of I and its Me ester (II) were independently determined on the basis of ROESY, NOESY, NOEDS, and Jvic evidence. By employing the same methods, the complete relative stereochem. was determined by anal. of suitable transformation products, using the reduced β-ketodihydropyrrole ring as a stereochem. bridge between the two zones. These results were confirmed by X-ray anal. of the 7-p-bromobenzoate Me ester derivative (III). The absolute stereochem. was established by application of the advanced Mosher method to II. Of biogenetic interest is the presence of a unique isoprenylated indole moiety not previously found in other indole mycotoxins.

IT ***196504-54-8P 196504-56-0P 196504-59-3P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of; isolation, structure determination, and chemical
transformations of nodulisporic acid A, an insecticide from a Nodulisporium Sp.)

RN 196504-54-8 CAPLUS

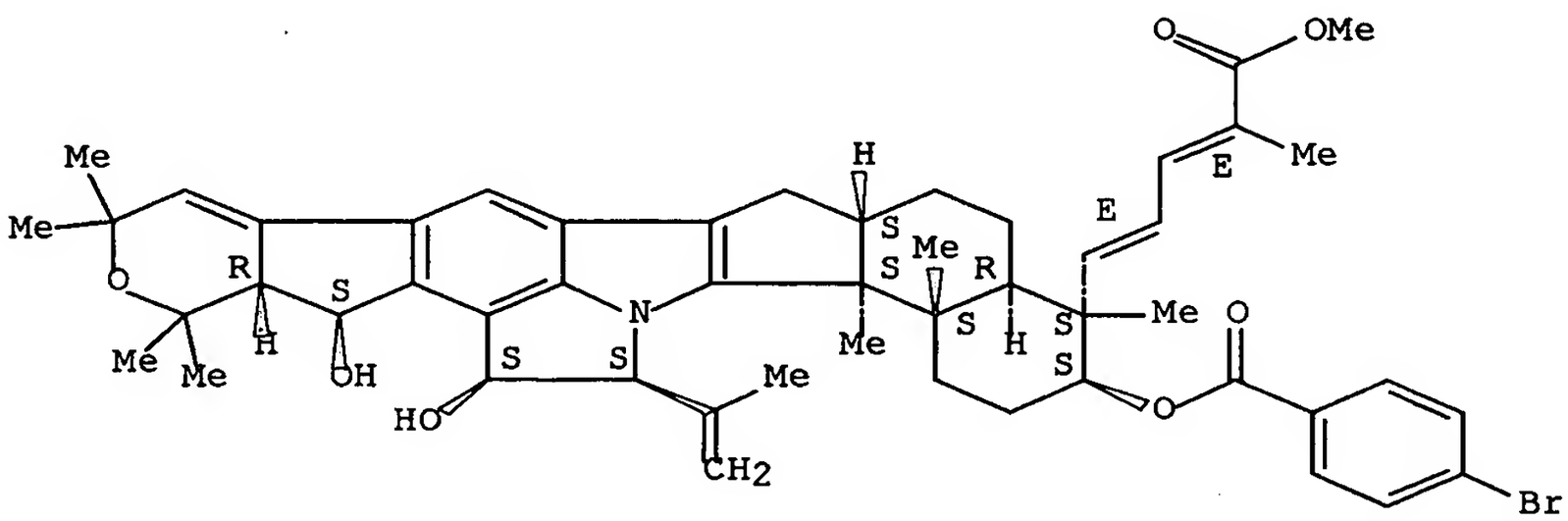
CN Benzoic acid, 4-bromo-, 2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-14-hydroxy-13-(methoxymethoxy)-4-(5-methoxy-4-methyl-5-oxo-1,3-pentadienyl)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-14-oxo-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-3-yl ester, [3S-[3α,4β(1E,3E),4aβ,6aα,12aα,13α,14α,15α,16bβ,16cα]]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



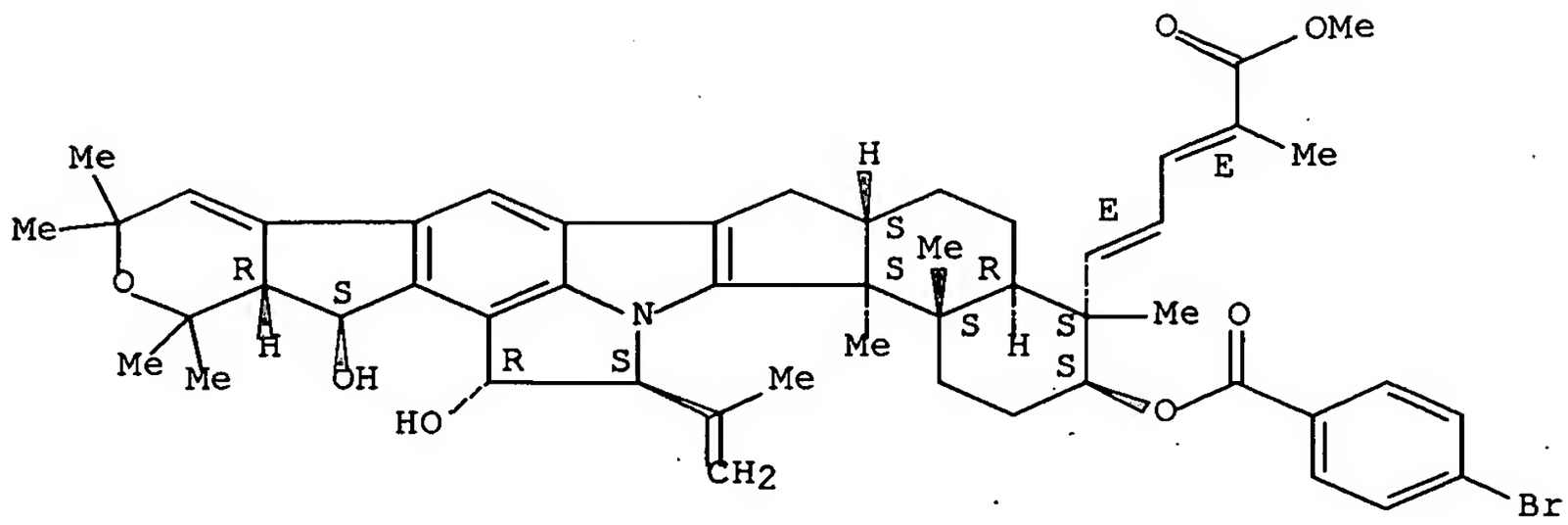
RN 196504-56-0 CAPLUS
CN Benzoic acid, 4-bromo-, 2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-13,14-dihydroxy-4-(5-methoxy-4-methyl-5-oxo-1,3-pentadienyl)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-14-oxo-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-3-yl ester, [3S-[3α,4β(1E,3E),4aβ,6aα,12a.alpha.,13α,14α,15α,16bβ,16cα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 196504-59-3 CAPLUS
CN Benzoic acid, 4-bromo-, 2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-13,14-dihydroxy-4-(5-methoxy-4-methyl-5-oxo-1,3-pentadienyl)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-14-oxo-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-3-yl ester, [3S-[3α,4β(1E,3E),4aβ,6aα,12a.alpha.,13α,14β,15α,16bβ,16cα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:689452 CAPLUS Full-text
DOCUMENT NUMBER: 125:328391
TITLE: Nodulisporic acid derivatives
INVENTOR(S): Meinke, Peter T.; Shih, Thomas; Fisher, Michael H.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9629073	A1	19960926	WO 1996-US3611	19960315
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2215982	A1	19960926	CA 1996-2215982	19960315
CA 2215982	C	20010612		
AU 9653134	A	19961008	AU 1996-53134	19960315
AU 691424	B2	19980514		
EP 819000	A1	19980121	EP 1996-909730	19960315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI				
JP 10504041	T	19980414	JP 1996-528529	19960315
JP 3020279	B2	20000315		
CN 1184423	A	19980610	CN 1996-193987	19960315
CN 1082814	B	20020417		
BR 9607965	A	19980714	BR 1996-7965	19960315
HU 9801749	A2	19981130	HU 1998-1749	19960315
PL 185563	B1	20030630	PL 1996-322326	19960315
CZ 294699	B6	20050216	CZ 1997-2935	19960315
SK 284840	B6	20051201	SK 1997-1259	19960315
ZA 9602203	A	19960904	ZA 1996-2203	19960319
TW 534908	B	20030601	TW 1996-85111484	19960919
NO 9704321	A	19971119	NO 1997-4321	19970919

PRIORITY APPLN. INFO.: US 1995-406619 A2 19950320
US 1996-606312 A2 19960311
WO 1996-US3611 W 19960315

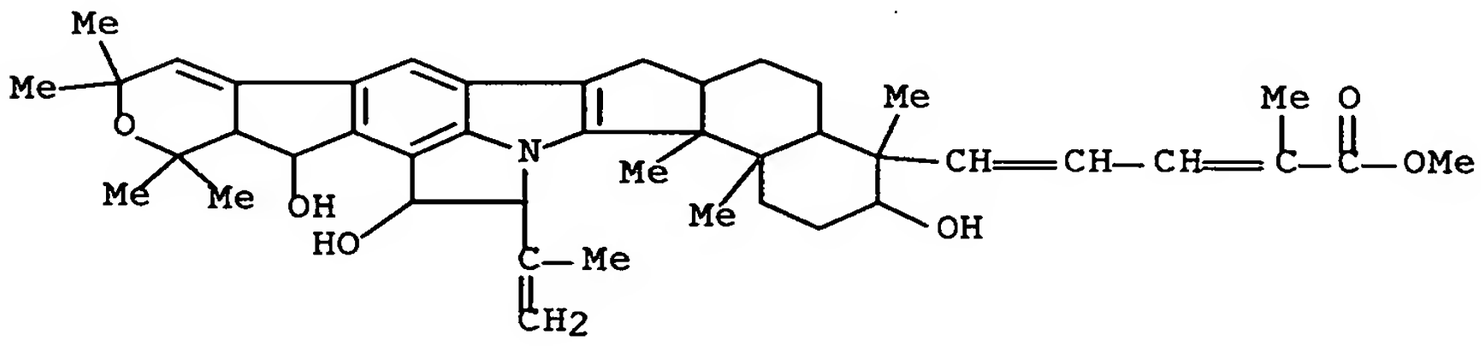
OTHER SOURCE(S): MARPAT 125:328391

AB Esters and amides of nodulisporic acid, 29,30-dihydro-20,30- oxanodulisporic acid and 31-hydroxy-20,30-oxa-29,30,31,32- tetrahydronudulic acid (>300 compds.), which are acaricidal, antiparasitic, insecticidal and anthelmintic agents (no data), were prepared Thus, nodulisporic acid was esterified with Me3SiCHN2 to give the Me ester.

IT ***183161-19-5P***, Methyl 1-hydroxynodulisporate ***183161-20-8P*** ***183161-26-4P***, 1-Hydroxynodulisporic acid ***183161-28-6P*** ***183161-29-7P*** ***183287-41-4P*** ***183287-44-7P*** ***183287-45-8P***
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nodulisporic acid esters and amides as parasiticides)

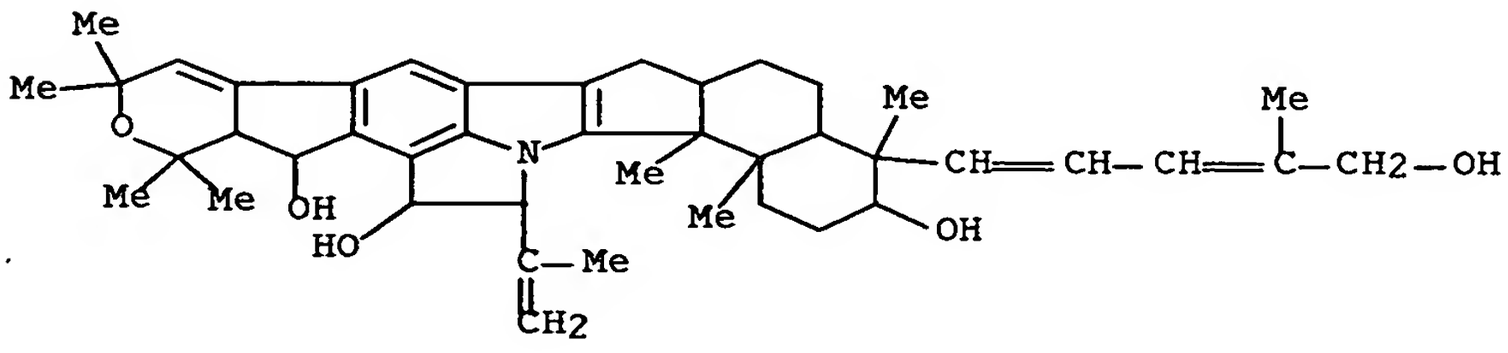
RN 183161-19-5 CAPLUS

CN 2,4-Pentadienoic acid, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-, methyl ester, [3S-[3α,4β(2E,4E),4aβ,6aα,12aα,13α,14.beta.,15α,16bβ,16cα]]- (9CI) (CA INDEX NAME)



RN 183161-20-8 CAPLUS

CN 1H-Benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indole-3,13,14-triol, 2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-4-(5-hydroxy-4-methyl-1,3-pentadienyl)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)- (9CI) (CA INDEX NAME)



RN 183161-26-4 CAPLUS

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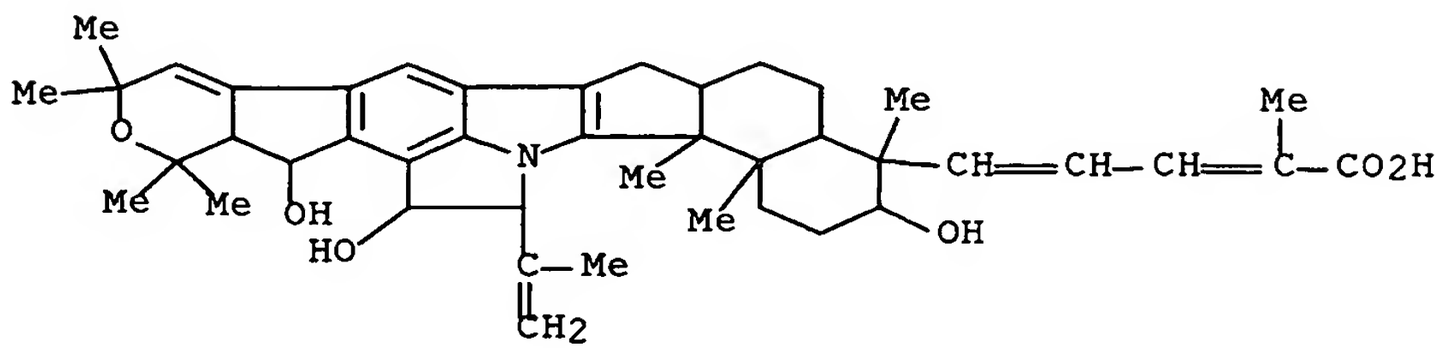
[3α,4β(2E,4E),4aβ,6aα,12aα,13α,14β,
15α,16bβ,16cα]]- (9CI) (CA INDEX NAME)



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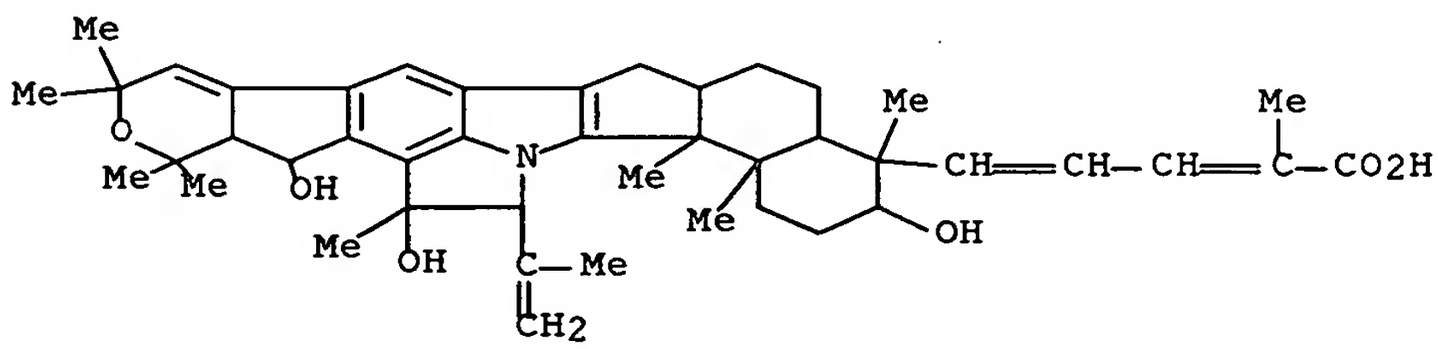
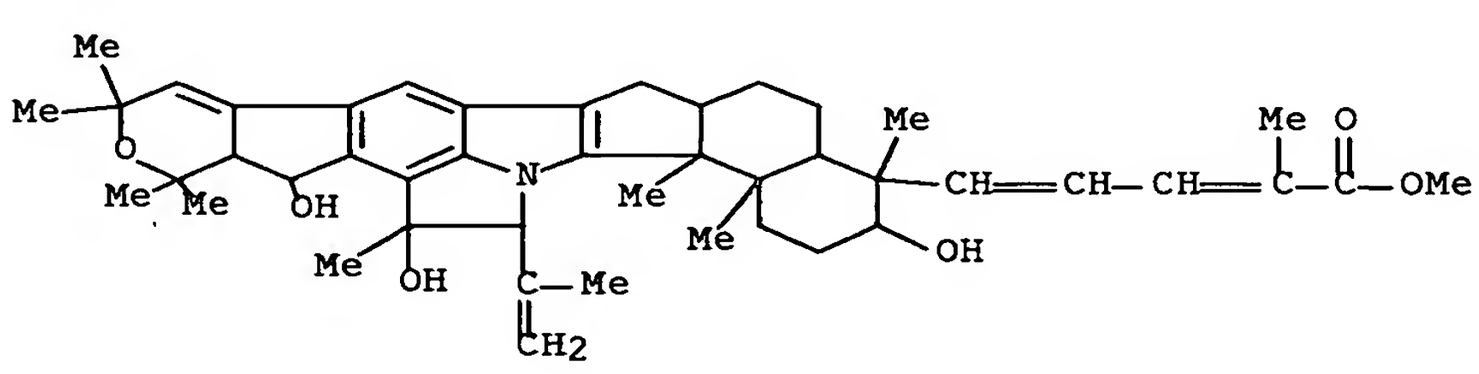
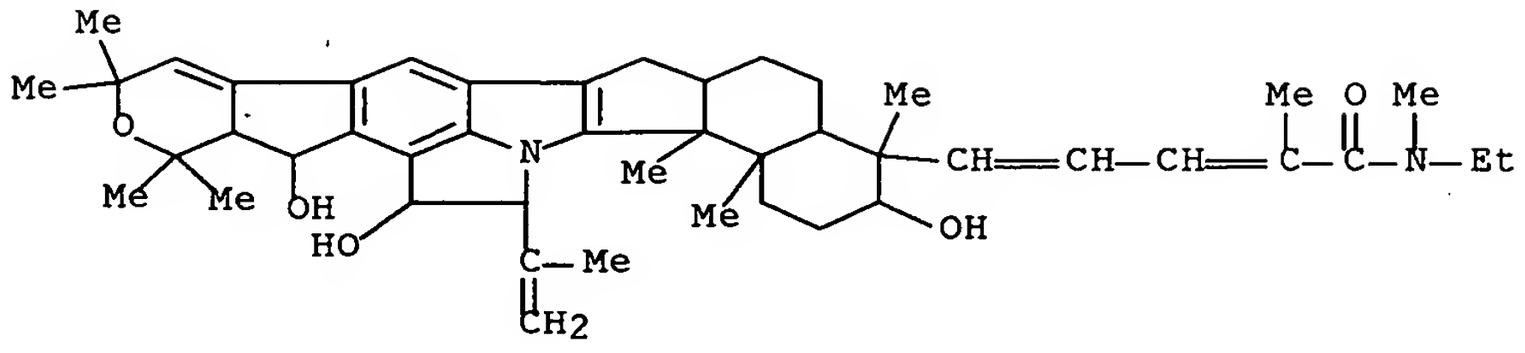


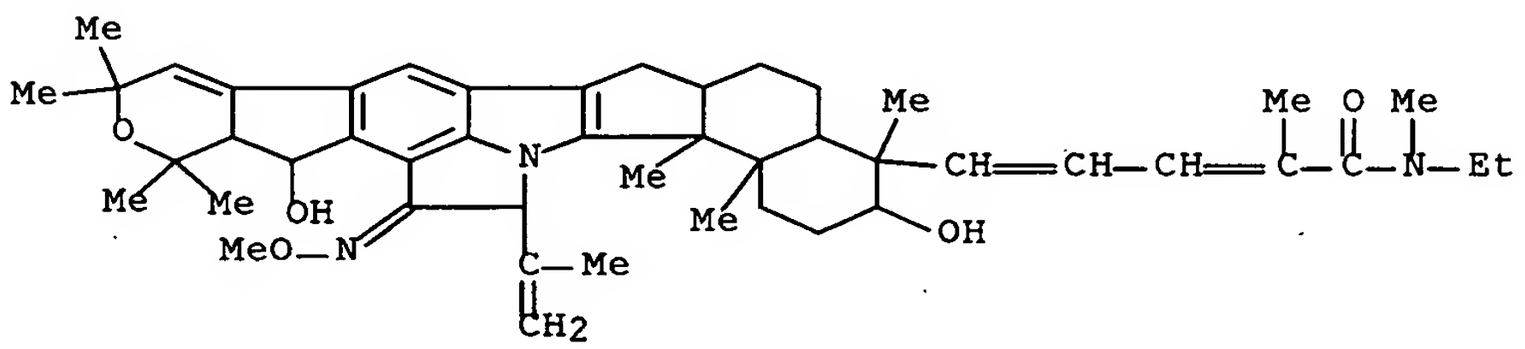
RN 183161-29-7 CAPLUS
CN 2,4-Pentadienoic acid, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,14,16b,16c-octamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



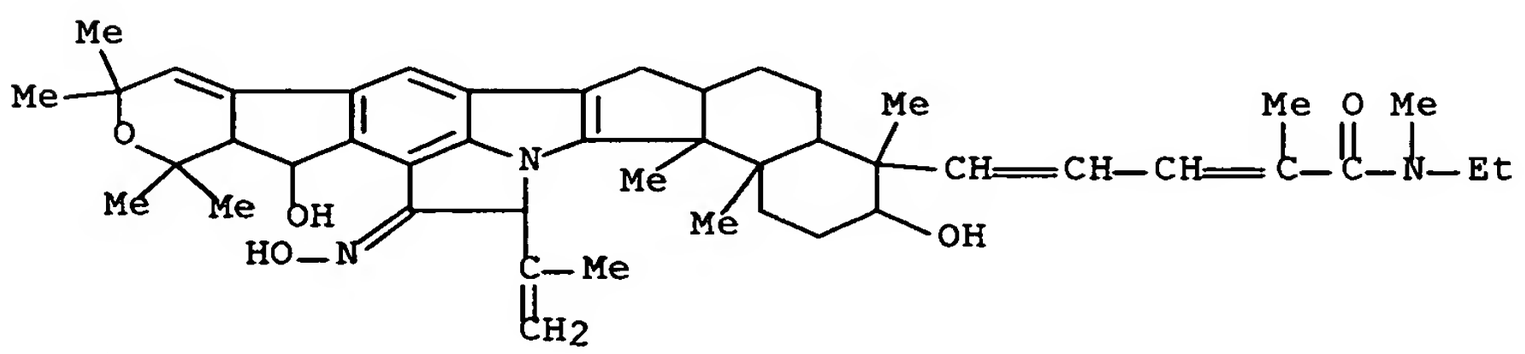
RN 183287-41-4 CAPLUS
CN 2,4-Pentadienamide, N-ethyl-5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-N,2-dimethyl- (9CI) (CA INDEX NAME)



RN 183287-44-7 CAPLUS
CN 2,4-Pentadienamide, N-ethyl-5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13-dihydroxy-14-(methoxyimino)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-N,2-dimethyl- (9CI) (CA INDEX NAME)



RN 183287-45-8 CAPLUS
CN 2,4-Pentadienamide, N-ethyl-5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13-dihydroxy-14-(hydroxyimino)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-N,2-dimethyl- (9CI) (CA INDEX NAME)

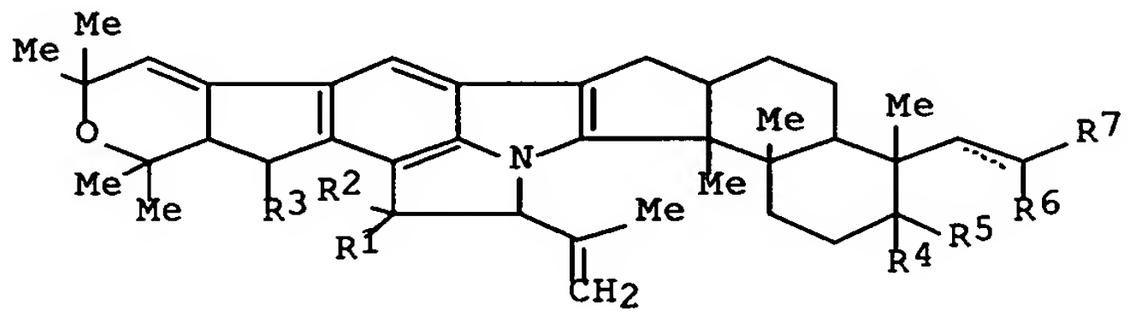


L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:679305 CAPLUS Full-text
DOCUMENT NUMBER: 125:328392
TITLE: Anthelmintic use of nodulisporic acid and analogs thereof
INVENTOR(S): Shoop, Wesley; Ostlind, Dan A.; Michael, Bruce F.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA

SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9629072	A1	19960926	WO 1996-US3598	19960315
W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5595991	A	19970121	US 1995-406447	19950320
AU 9652542	A	19961008	AU 1996-52542	19960315
ZA 9602202	A	19960926	ZA 1996-2202	19960319
PRIORITY APPLN. INFO.:			US 1995-406447	A1 19950320
			WO 1996-US3598	W 19960315

OTHER SOURCE(S): MARPAT 125:328392
GI

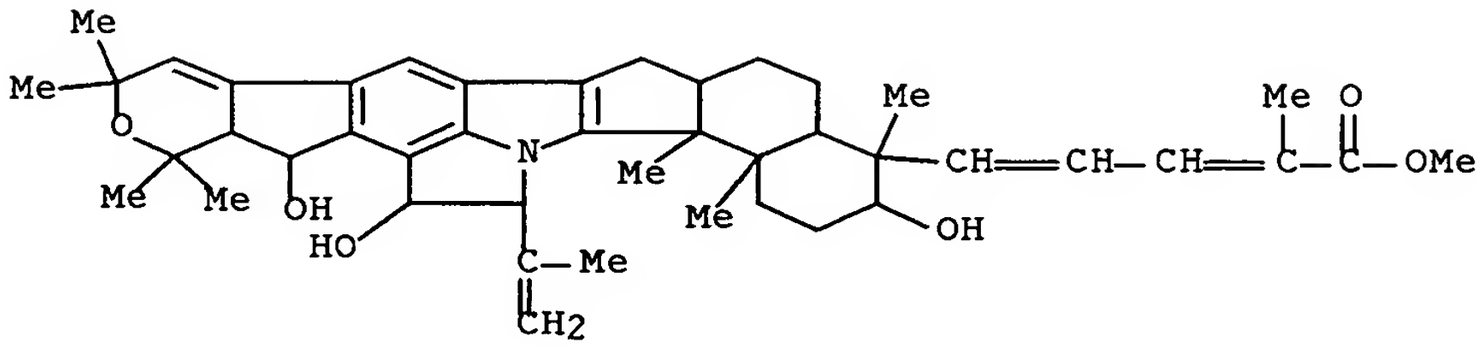


I

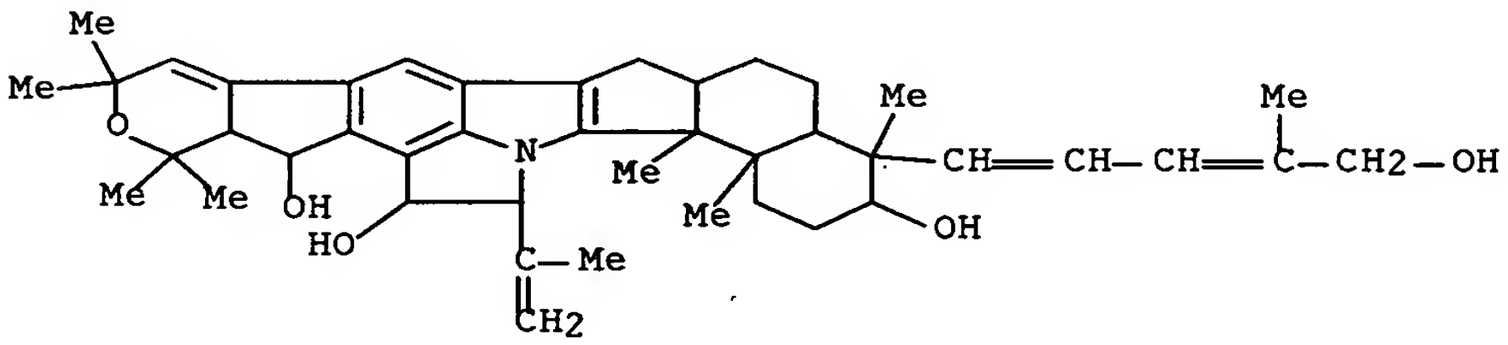
AB The present invention provides a method for the treatment of helminthiasis which comprises administering to an infected host an effective amount of a nodulisporic acid analog I [R1 = H, (un)substituted aliphatic, cycloaliph., heterocyclic, aryl; R2, R3, R4 = (un)substituted OH; R1R2 = O, (un)substituted NO NOH, NNH2; R5R6 = H2, O; R7 = CHO, (un)substituted aliphatic]. Some derivs. of I [R1R2 = O, R3, R4 = OH, R5, R6 = H, R5R6 = O, R7 = CH:CMeCO2H, CH(OH)CHMeCO2H; the dotted bond is single or double] were prepared

IT ***183161-19-5P 183161-20-8P 183161-26-4P,***
1-Hydroxynodulisporic acid ***183161-28-6P,*** 1-Hydroxy-1-methylnodulisporic acid ***183161-29-7P***
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and anthelmintic use of nodulisporic acid analogs)

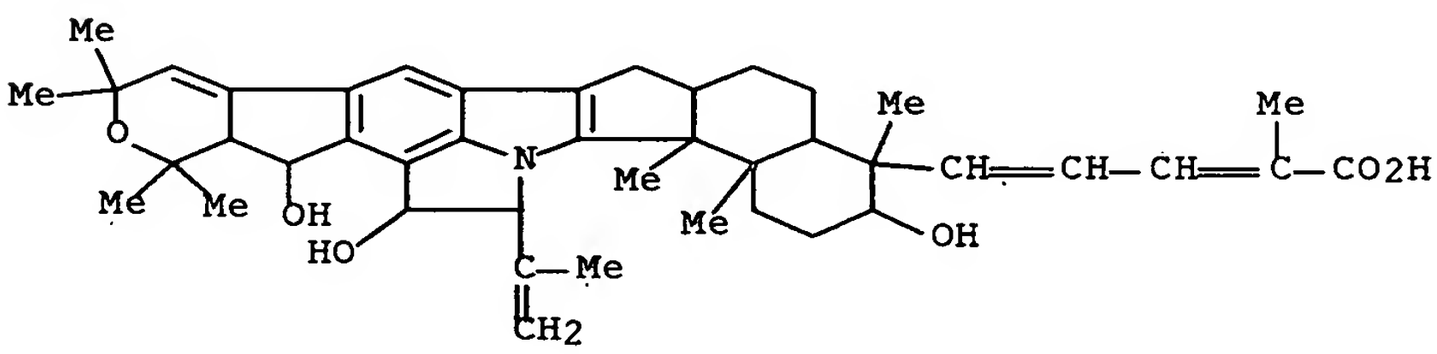
RN 183161-19-5 CAPLUS
CN 2,4-Pentadienoic acid, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-, methyl ester, [3S-[3α,4β(2E,4E),4aβ,6aα,12aα,13α,14.beta.,15α,16bβ,16cα]]- (9CI) (CA INDEX NAME)



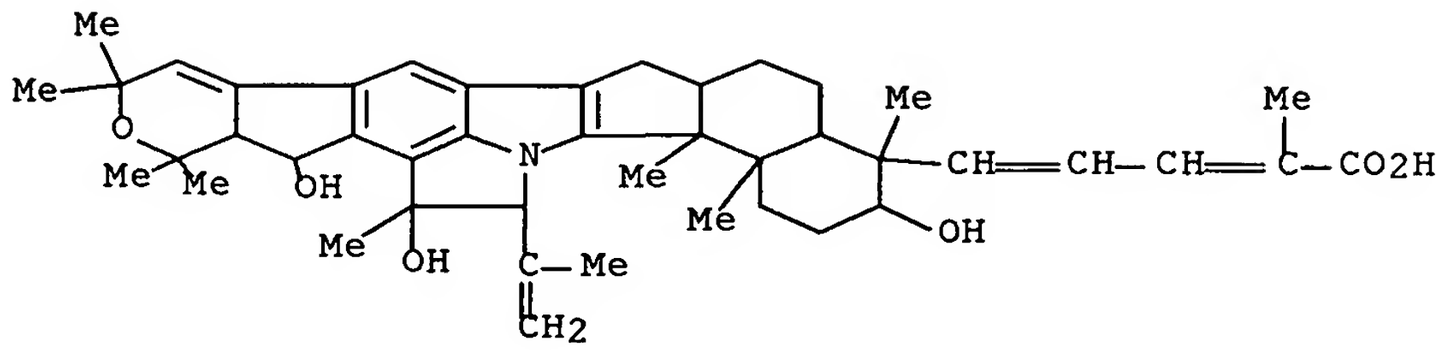
RN 183161-20-8 CAPLUS
CN 1H-Benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indole-3,13,14-triol, 2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-4-(5-hydroxy-4-methyl-1,3-pentadienyl)-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)- (9CI) (CA INDEX NAME)



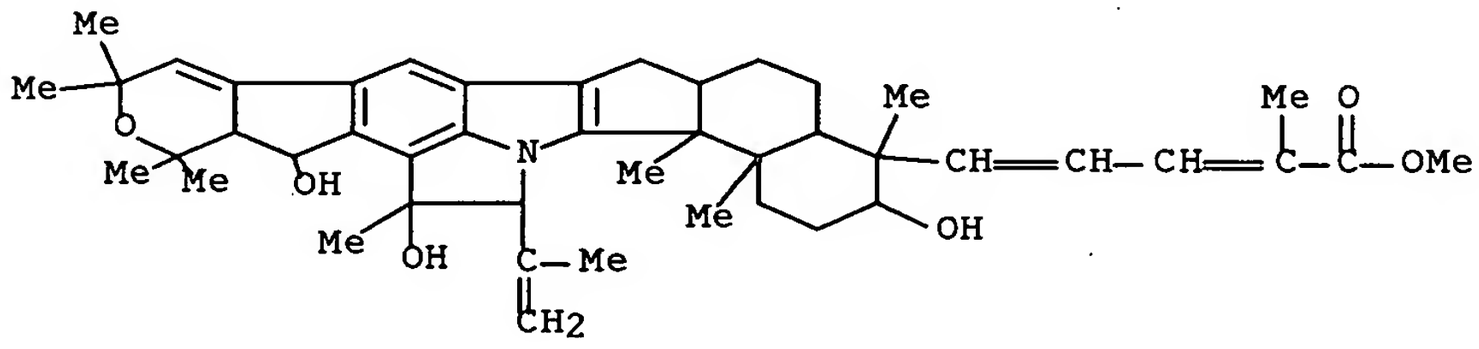
RN 183161-26-4 CAPLUS
CN 2,4-Pentadienoic acid, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,16b,16c-heptamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-, [3S-[3α,4β(2E,4E),4aβ,6aα,12aα,13α,14β,15α,16bβ,16cα]]- (9CI) (CA INDEX NAME)



RN 183161-28-6 CAPLUS
CN 2,4-Pentadienoic acid, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,14,16b,16c-octamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl- (9CI) (CA INDEX NAME)



RN 183161-29-7 CAPLUS
CN 2,4-Pentadienoic acid, 5-[2,3,4,4a,5,6,6a,7,10,12,12a,13,14,15,16b,16c-hexadecahydro-3,13,14-trihydroxy-4,10,10,12,12,14,16b,16c-octamethyl-15-(1-methylethenyl)-1H-benz[6,7]indeno[1,2-b]pyrano[3',4':4,5]cyclopenta[1,2-f]pyrrolo[3,2,1-hi]indol-4-yl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)



=> fil beilst
FILE 'BEILSTEIN' ENTERED AT 12:43:32 ON 16 FEB 2007
COPYRIGHT (c) 2007 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON JANUARY 10, 2007

FILE COVERS 1771 TO 2006.
*** FILE CONTAINS 9,780,003 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *

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* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
**********************************************************************
```

NEW

**** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.***

**** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.***

```
=> d que l7
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str
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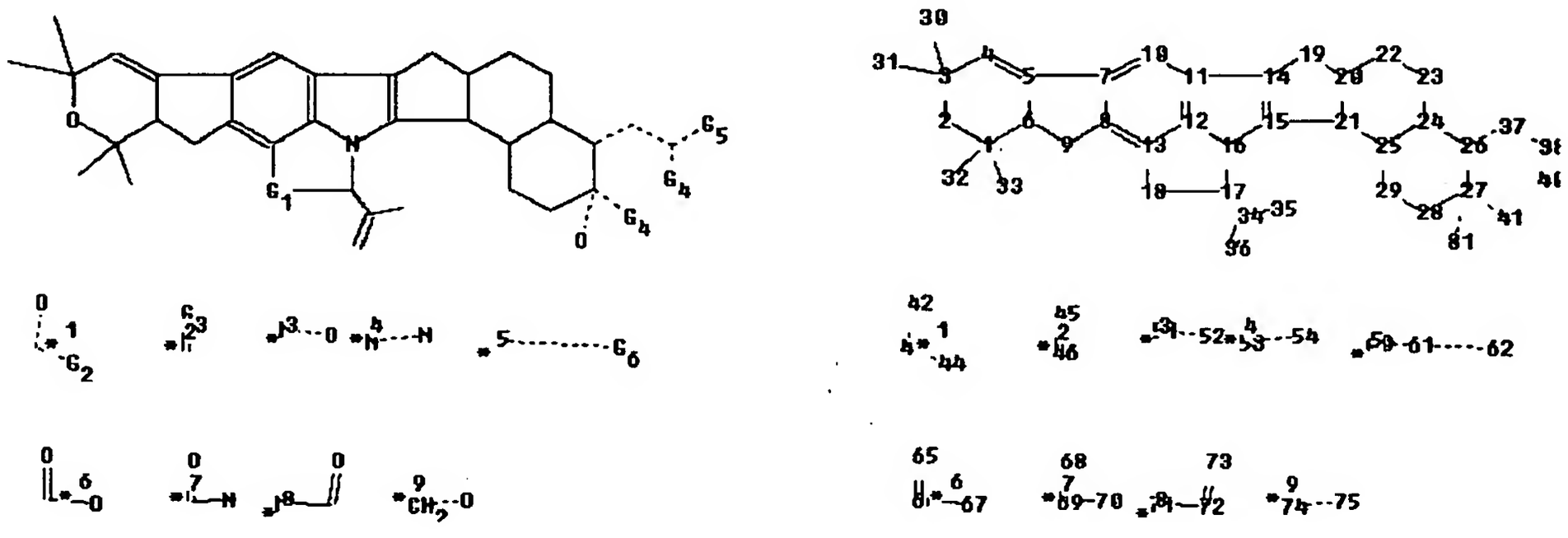

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chain nodes :
30  31  32  33  34  35  36  39  40  41  42  43  44  45  46  51  52  53  54  60  61
62  65  66  67  68  69  73  74  75  81
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22  23
24  25  26  27  28  29
ring/chain nodes :
37  38  70  71  72
chain bonds :
1-32  1-33  3-30  3-31  17-34  27-81  34-35  34-36  38-39  42-43  43-44  45-46  51-
52
53-54  60-61  61-62  65-66  66-67  68-69  69-70  72-73  74-75
ring/chain bonds :
26-37  27-41  37-38  38-40  71-72
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  7-10  8-9  8-13  10-11  11-12  11-14
```

```
12-13  12-16  13-18  14-15  14-19  15-16  15-21  16-17  17-18  19-20  20-21  20-22
21-25  22-23
23-24  24-25  24-26  25-29  26-27  27-28  28-29
exact/norm bonds :
1-2  1-6  1-32  1-33  2-3  3-4  3-30  3-31  4-5  5-6  5-7  6-9  8-9  11-14  12-16
13-18  14-15  14-19  15-16  15-21  16-17  17-18  17-34  19-20  20-21  20-22  21-25
22-23  23-24
24-25  24-26  25-29  26-27  26-37  27-28  27-41  27-81  28-29  34-35  34-36  37-38
38-39  38-40
42-43  43-44  45-46  51-52  53-54  60-61  61-62  65-66  66-67  68-69  69-70  71-72
72-73  74-75
normalized bonds :
7-8  7-10  8-13  10-11  11-12  12-13

G1:[*1],[*2]

G2:H,Cy,Ak

G3:[*3],[*4]

G4:H,O

G5:CHO,[*5]

G6:CN,[*6],[*7],[*8],[*9]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
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22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:CLASS
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43:CLASS  44:CLASS  45:CLASS  46:CLASS  51:CLASS  52:CLASS  53:CLASS  54:CLASS
60:CLASS  61:CLASS
62:CLASS  65:CLASS  66:CLASS  67:CLASS  68:CLASS  69:CLASS  70:CLASS  71:CLASS
72:CLASS  73:CLASS
74:CLASS  75:CLASS  81:CLASS
```

```
L6              5 SEA FILE=BEILSTEIN SSS FUL L1
L7              5 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L6 NOT RN/FA


=> d que l9
L1                STR

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Structure attributes must be viewed using STN Express query preparation:

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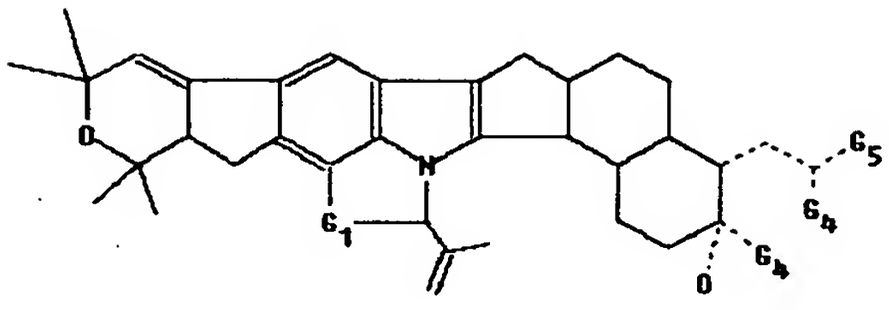
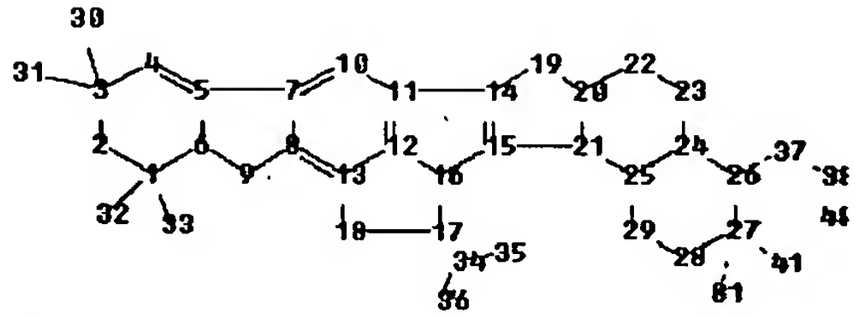
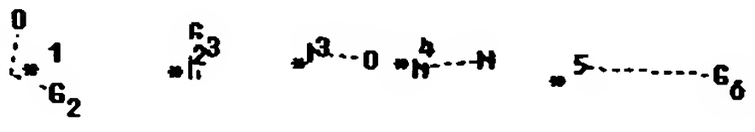
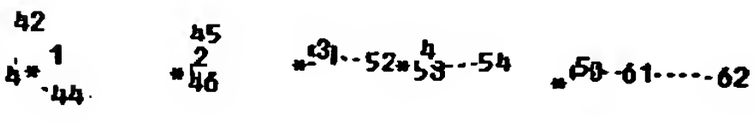
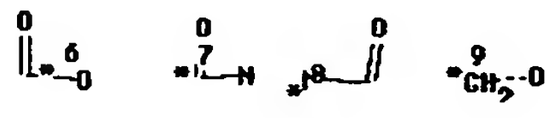
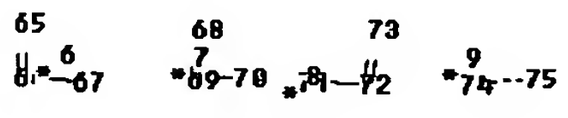












chain nodes :
30 31 32 33 34 35 36 39 40 41 42 43 44 45 46 51 52 53 54 60 61
62 65 66 67 68 69 73 74 75 81
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29
ring/chain nodes :
37 38 70 71 72
chain bonds :
1-32 1-33 3-30 3-31 17-34 27-81 34-35 34-36 38-39 42-43 43-44 45-46 51-
52
53-54 60-61 61-62 65-66 66-67 68-69 69-70 72-73 74-75
ring/chain bonds :
26-37 27-41 37-38 38-40 71-72
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 7-10 8-9 8-13 10-11 11-12 11-14
12-13 12-16 13-18 14-15 14-19 15-16 15-21 16-17 17-18 19-20 20-21 20-22
21-25 22-23
23-24 24-25 24-26 25-29 26-27 27-28 28-29
exact/norm bonds :
1-2 1-6 1-32 1-33 2-3 3-4 3-30 3-31 4-5 5-6 5-7 6-9 8-9 11-14 12-16
13-18 14-15 14-19 15-16 15-21 16-17 17-18 17-34 19-20 20-21 20-22 21-25
22-23 23-24
24-25 24-26 25-29 26-27 26-37 27-28 27-41 27-81 28-29 34-35 34-36 37-38
38-39 38-40
42-43 43-44 45-46 51-52 53-54 60-61 61-62 65-66 66-67 68-69 69-70 71-72
72-73 74-75
normalized bonds :
7-8 7-10 8-13 10-11 11-12 12-13

G1:[*1],[*2]

G2:H,Cy,Ak

G3:[*3],[*4]

G4:H,O

G5:CHO,[*5]

G6:CN,[*6],[*7],[*8],[*9]

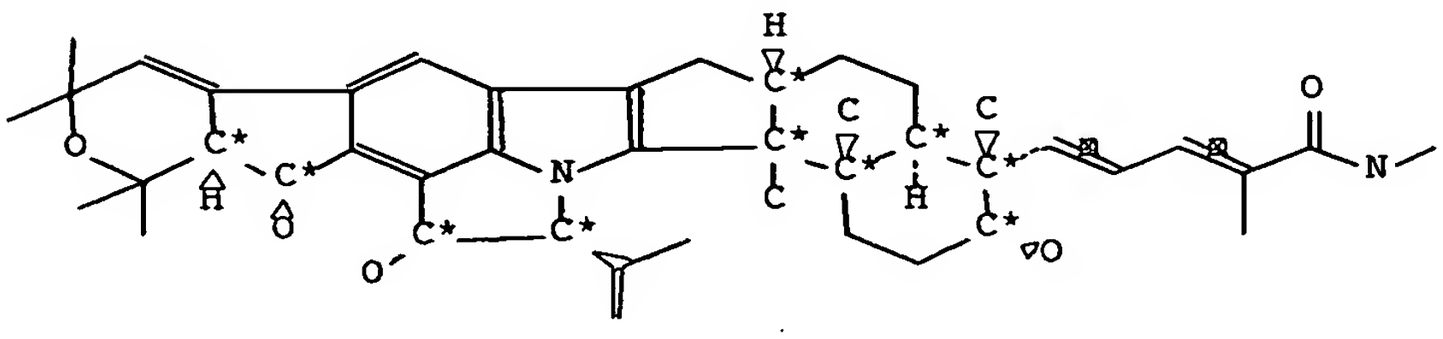
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:CLASS
31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS
43:CLASS 44:CLASS 45:CLASS 46:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS
60:CLASS 61:CLASS
62:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS
72:CLASS 73:CLASS
74:CLASS 75:CLASS 81:CLASS

L6 5 SEA FILE=BEILSTEIN SSS FUL L1
L7 5 SEA FILE=BEILSTEIN ABB=ON PLU=ON L6 NOT RN/FA
L8 4 SEA FILE=BEILSTEIN ABB=ON PLU=ON L6 AND BABSAN/FA
L9 1 SEA FILE=BEILSTEIN ABB=ON PLU=ON L7 NOT L8

=> d l9 ide allref

L9 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	8751109
Molec. Formula (MF):	C44 H58 N2 O5
Molecular Weight (MW):	694.95
Lawson Number (LN):	31479, 2817
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7408918
Tautomer ID (TAUTID):	8230199
Entry Date (DED):	2001/04/26
Update Date (DUPD):	2001/04/26



Field Availability:

Code	Name	Occurrence
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MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

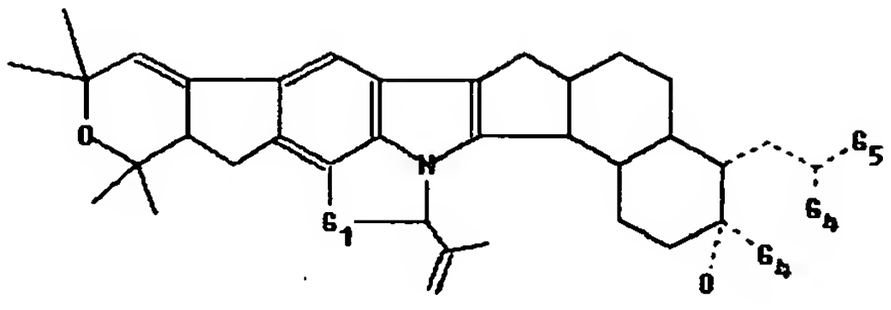
1. Meinke, Peter T.; Ayer, Michelle B.; Colletti, Steven L.; Li, Chunshi; Lim, Julie; Ok, Dong; Salva, Steve; Schmatz, Dennis M.; Shih, Thomas L.; Shoop, Wesley L.; Warmke, Lynn M.; et al., Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 10(20), <2000>, 2371 - 2374; BABS-6266733

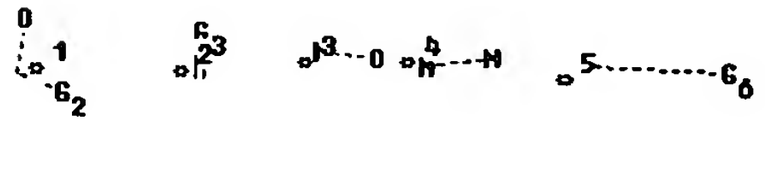
=> d que l11
L1 STR

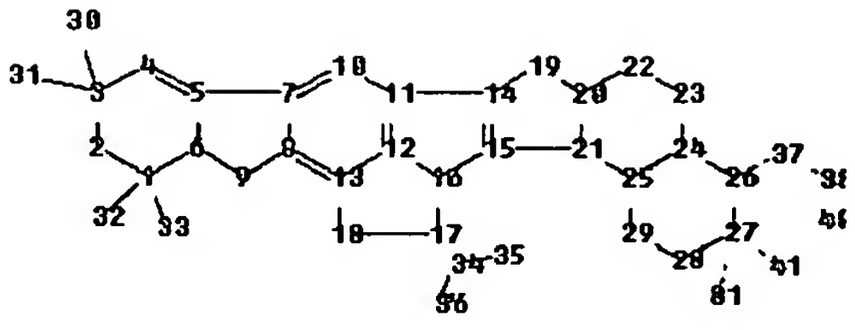
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

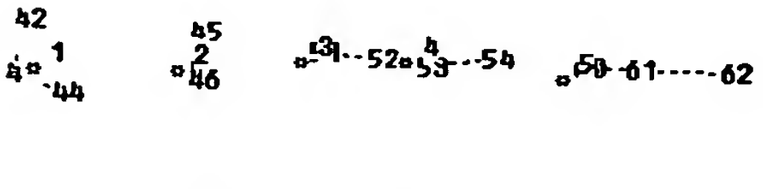
Structure attributes must be viewed using STN Express query preparation:

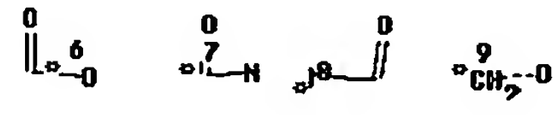
Uploading L1.str

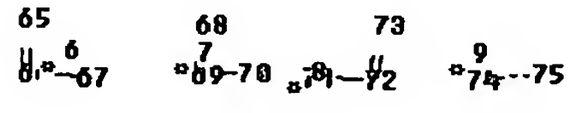












chain nodes :
30 31 32 33 34 35 36 39 40 41 42 43 44 45 46 51 52 53 54 60 61
62 65 66 67 68 69 73 74 75 81
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29
ring/chain nodes :
37 38 70 71 72
chain bonds :
1-32 1-33 3-30 3-31 17-34 27-81 34-35 34-36 38-39 42-43 43-44 45-46 51-
52
53-54 60-61 61-62 65-66 66-67 68-69 69-70 72-73 74-75
ring/chain bonds :
26-37 27-41 37-38 38-40 71-72
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 7-10 8-9 8-13 10-11 11-12 11-14
12-13 12-16 13-18 14-15 14-19 15-16 15-21 16-17 17-18 19-20 20-21 20-22
21-25 22-23
23-24 24-25 24-26 25-29 26-27 27-28 28-29
exact/norm bonds :
1-2 1-6 1-32 1-33 2-3 3-4 3-30 3-31 4-5 5-6 5-7 6-9 8-9 11-14 12-16
13-18 14-15 14-19 15-16 15-21 16-17 17-18 17-34 19-20 20-21 20-22 21-25
22-23 23-24
24-25 24-26 25-29 26-27 26-37 27-28 27-41 27-81 28-29 34-35 34-36 37-38
38-39 38-40
42-43 43-44 45-46 51-52 53-54 60-61 61-62 65-66 66-67 68-69 69-70 71-72
72-73 74-75
normalized bonds :
7-8 7-10 8-13 10-11 11-12 12-13

G1:[*1],[*2]

G2:H,Cy,Ak

G3:[*3],[*4]

G4:H,O

G5:CHO,[*5]

G6:CN,[*6],[*7],[*8],[*9]

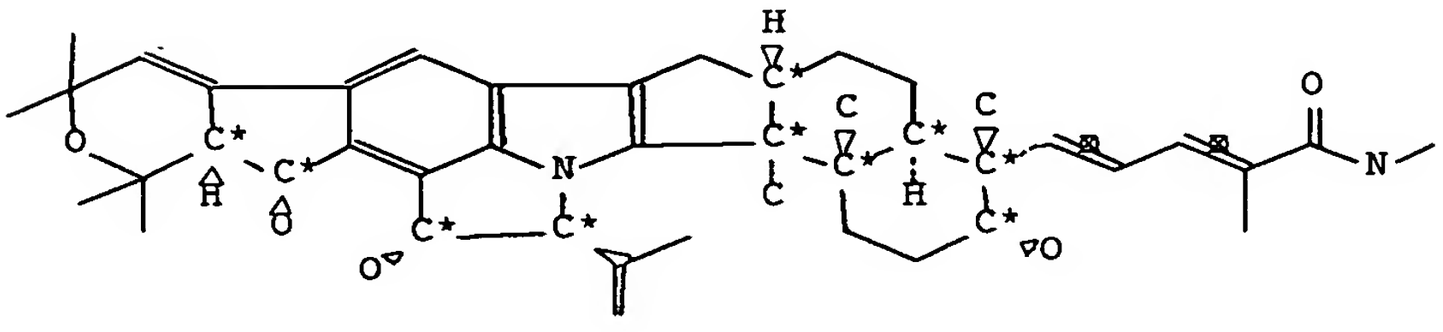
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:CLASS
31:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS
43:CLASS 44:CLASS 45:CLASS 46:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS
60:CLASS 61:CLASS
62:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS
72:CLASS 73:CLASS
74:CLASS 75:CLASS 81:CLASS

L6 5 SEA FILE=BEILSTEIN SSS FUL L1
L8 4 SEA FILE=BEILSTEIN ABB=ON PLU=ON L6 AND BABSAN/FA
L11 1 SEA FILE=BEILSTEIN ABB=ON PLU=ON L8 AND 6266733/BABSAN

=> d l11 ide allref

L11 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	8751110
Molec. Formula (MF):	C44 H58 N2 O5
Molecular Weight (MW):	694.95
Lawson Number (LN):	31479, 2817
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7408918
Tautomer ID (TAUTID):	8230200
Entry Date (DED):	2001/04/26
Update Date (DUPD):	2001/04/26



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
DED	Entry Date	1
DUPD	Update Date	1
PHARM	Pharmacological Data	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

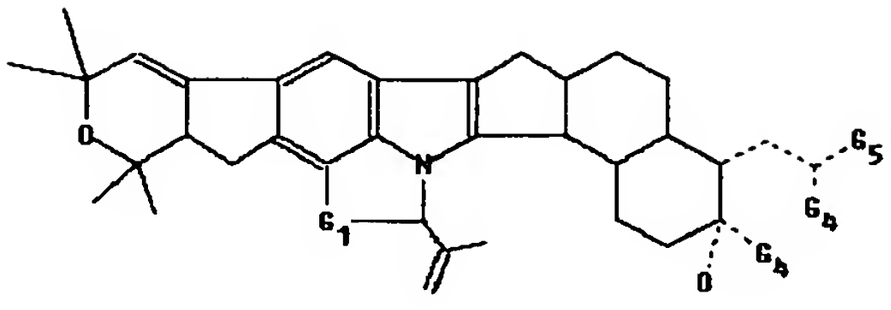
1. Meinke, Peter T.; Ayer, Michelle B.; Colletti, Steven L.; Li, Chunshi; Lim, Julie; Ok, Dong; Salva, Steve; Schmatz, Dennis M.; Shih, Thomas L.; Shoop, Wesley L.; Warmke, Lynn M.; et al., Bioorg.Med.Chem.Lett., CODEN: BMCLE8, 10(20), <2000>, 2371 - 2374; BABS-6266733

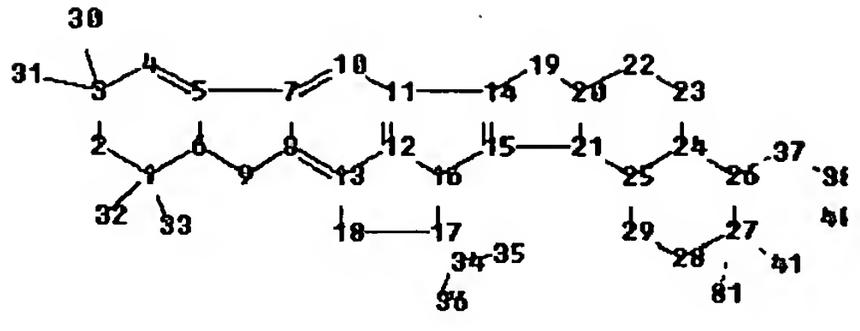
=> d que l12
L1 STR

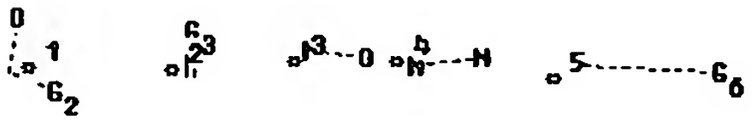
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

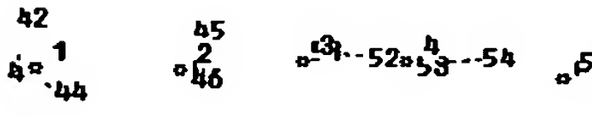
Structure attributes must be viewed using STN Express query preparation:

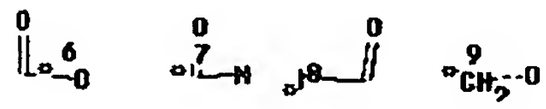
Uploading L1.str

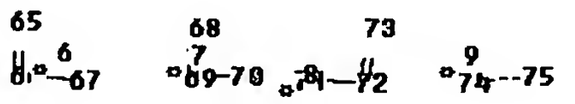












chain nodes :
30 31 32 33 34 35 36 39 40 41 42 43 44 45 46 51 52 53 54 60 61
62 65 66 67 68 69 73 74 75 81
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29
ring/chain nodes :
37 38 70 71 72
chain bonds :
1-32 1-33 3-30 3-31 17-34 27-81 34-35 34-36 38-39 42-43 43-44 45-46 51-
52
53-54 60-61 61-62 65-66 66-67 68-69 69-70 72-73 74-75
ring/chain bonds :
26-37 27-41 37-38 38-40 71-72
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 7-10 8-9 8-13 10-11 11-12 11-14
12-13 12-16 13-18 14-15 14-19 15-16 15-21 16-17 17-18 19-20 20-21 20-22
21-25 22-23
23-24 24-25 24-26 25-29 26-27 27-28 28-29
exact/norm bonds :
1-2 1-6 1-32 1-33 2-3 3-4 3-30 3-31 4-5 5-6 5-7 6-9 8-9 11-14 12-16
13-18 14-15 14-19 15-16 15-21 16-17 17-18 17-34 19-20 20-21 20-22 21-25
22-23 23-24
24-25 24-26 25-29 26-27 26-37 27-28 27-41 27-81 28-29 34-35 34-36 37-38
38-39 38-40
42-43 43-44 45-46 51-52 53-54 60-61 61-62 65-66 66-67 68-69 69-70 71-72
72-73 74-75
normalized bonds :
7-8 7-10 8-13 10-11 11-12 12-13

G1:[*1],[*2]

G2:H,Cy,Ak

```
G3:[*3],[*4]

G4:H,O

G5:CHO,[*5]

G6:CN,[*6],[*7],[*8],[*9]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
20:Atom  21:Atom
22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:CLASS
31:CLASS  32:CLASS
33:CLASS  34:CLASS  35:CLASS  36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS
41:CLASS  42:CLASS
43:CLASS  44:CLASS  45:CLASS  46:CLASS  51:CLASS  52:CLASS  53:CLASS  54:CLASS
60:CLASS  61:CLASS
62:CLASS  65:CLASS  66:CLASS  67:CLASS  68:CLASS  69:CLASS  70:CLASS  71:CLASS
72:CLASS  73:CLASS
74:CLASS  75:CLASS  81:CLASS


L6              5 SEA FILE=BEILSTEIN SSS FUL L1
L8              4 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L6 AND BABSAN/FA
L12             3 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L8 AND 6080270/BABSAN


=> d l12 ide allref 1


L12  ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

     Beilstein Records (BRN):          7903768
     Chemical Name (CN):               7-(p-bromobenzoyl)-1'β-
                                       hydroxynodulisporic acid A
     Molec. Formula (MF):              C51 H60 Br N O7
     Molecular Weight (MW):            878.94
     Lawson Number (LN):               31479, 10582, 289
     File Segment (FS):                Stereo compound
     Compound Type (CTYPE):            heterocyclic
     Constitution ID (CONSID):         6743985
     Tautomer ID (TAUTID):             7479665
     Beilstein Citation (BSO):         6-27
     Entry Date (DED):                 1998/07/15
     Update Date (DUPD):               1998/07/15
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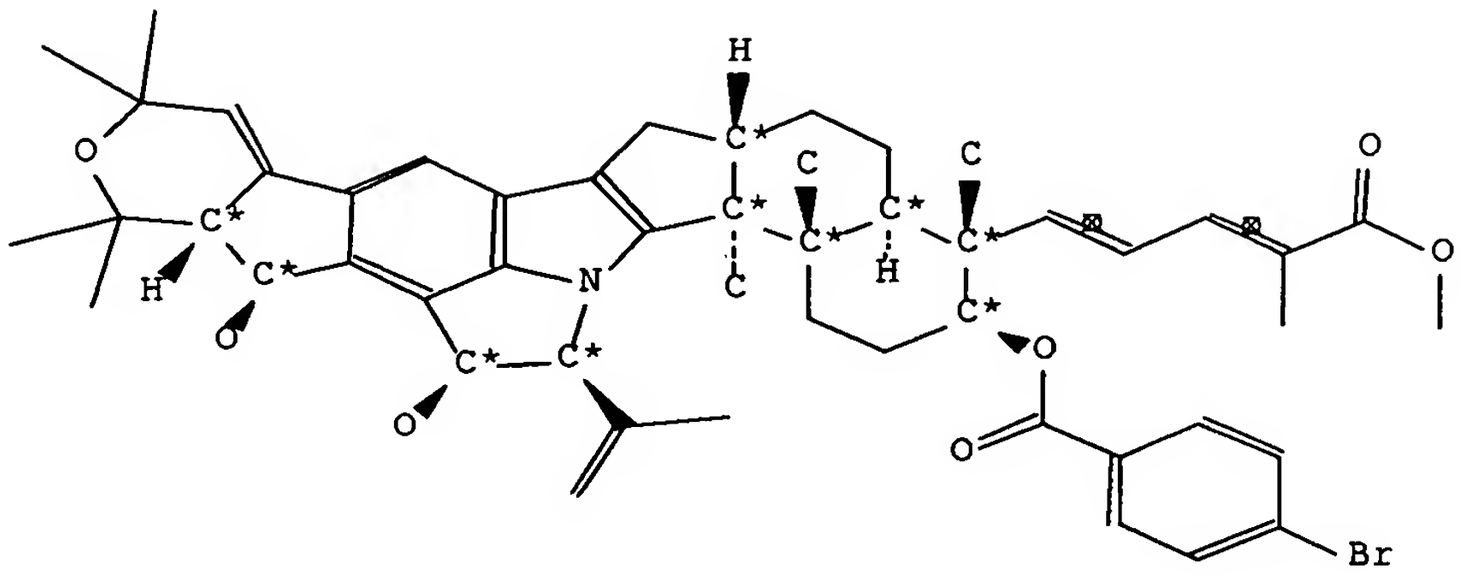

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Ondeyka, John G.; Helms, Gregory L.; Hensens, Otto D.; Goetz, Michael A.; Zink, Deborah L.; et al., J.Amer.Chem.Soc., CODEN: JACSAT, 119(38), <1997>, 8809-8816; BABS-6080270

HISTORY

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=> d his nofil

     (FILE 'HOME' ENTERED AT 11:16:18 ON 16 FEB 2007)

     FILE 'REGISTRY' ENTERED AT 11:20:57 ON 16 FEB 2007
L*** DEL          STR
L1                STRUCTURE UPLOADED
                  D
L2              1 SEA SSS SAM L1
                  D SCA
L3             13 SEA SSS FUL L1

     FILE 'CAPLUS' ENTERED AT 11:49:25 ON 16 FEB 2007
L4              5 SEA ABB=ON  PLU=ON  L3

     FILE 'MARPAT' ENTERED AT 11:49:35 ON 16 FEB 2007

     FILE 'BEILSTEIN' ENTERED AT 11:49:54 ON 16 FEB 2007
L5              0 SEA SSS SAM L1
L6              5 SEA SSS FUL L1
L7              5 SEA ABB=ON  PLU=ON  L6 NOT RN/FA
L8              4 SEA ABB=ON  PLU=ON  L6 AND BABSAN/FA
L9              1 SEA ABB=ON  PLU=ON  L7 NOT L8
                  SEL BABSAN L8

     FILE 'BABS' ENTERED AT 11:51:13 ON 16 FEB 2007
L10             2 SEA ABB=ON  PLU=ON  (6080270/AN OR 6266733/AN)
                  D 1-2
                  D COST

     FILE 'BEILSTEIN' ENTERED AT 11:53:26 ON 16 FEB 2007
L11             1 SEA ABB=ON  PLU=ON  L8 AND 6266733/BABSAN
L12             3 SEA ABB=ON  PLU=ON  L8 AND 6080270/BABSAN
L13               STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 12:39:40 ON 16 FEB 2007
L14             1 SEA SSS SAM L13
                  D SCA

     FILE 'MARPAT' ENTERED AT 12:39:51 ON 16 FEB 2007
L15               STRUCTURE UPLOADED

     FILE 'HCAPLUS' ENTERED AT 12:42:02 ON 16 FEB 2007
                  D QUE L4

     FILE 'CAPLUS' ENTERED AT 12:42:22 ON 16 FEB 2007
                  D QUE L4
                  D L4 IBIB ABS HITSTR TOT

     FILE 'BEILSTEIN' ENTERED AT 12:43:32 ON 16 FEB 2007
                  D QUE L7
                  D QUE L9
                  D L9 IDE ALLREF
                  D QUE L11
                  D L11 IDE ALLREF
                  D QUE L12
                  D L12 IDE ALLREF 1
```